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PATENTEE : LION CORP
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TITLE : AGENT FOR IMPARTING IRIDESCENT LUSTER TO COSMETIC

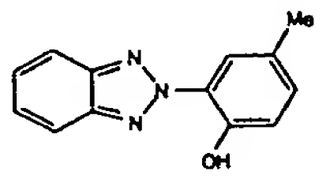
ABSTRACT : PURPOSE:To provide an agent for imparting excellent iridescent luster to cosmetics, and keeping the luster stably for a long period even at a high temperature, by using a straight-chain alkanediol diester as a main component.
CONSTITUTION:The objective iridescent luster agent contains at least one compound of formula (R and R' are 13-23C straight-chain alkyl; n is integer 3-10) pref. having a melting point of >=50 deg.C. The agent gives very beautiful and thermal- ly stable iridescent luster to liquid or pasty cosmetics such as shampoo, rinsing agent, lotion, cream, etc., by conventional compounding process. The use of a mixture of two or more kinds of the above compounds or the use of a compound wherein R is different from R' gives more desirable iridescent luster than the use of a compound wherein R is R'. Since larger molecular weight of R and R' results in higher melting point of the compound, desired thermal stability according to the purpose can be attained by selecting proper R and R'.

78186-34-2 9,10-Anthracenedicarboxaldehyde, bis[(4,5-dihydro-1*H*-imidazol-2-yl)hydrazone] $C_{22}H_{22}N_8$
78186-35-3 Iodine chloride (ICl_3) Cl_3I
78186-36-4 Propanoic acid, 2-methyl-, 2-(5-phenyl-1,2,4-triazin-3-yl)hydrazide, hydrochloride $C_{13}H_{15}N_5O.xClH$
78186-37-5 4-Piperidinecarboxamide, *N*-(2,6-dimethylphenyl)-1-methyl-, monohydrochloride $C_{15}H_{22}N_2O.ClH$
78186-38-6 Benzenemethanamine, 2,5-dimethoxy-α,α-dimethyl- $C_{11}H_{17}NO_2$
78186-39-7 Isoquinolinium, 2-[3-[4-[(hydroxyimino)methyl]pyridinio]propyl]-, dibromide $C_{18}H_{19}N_3O.2Br$
78186-40-0 Methanesulfonamide, *N*-[4-(9-acridinylamino)-3-methoxyphenyl]-, methanesulfonate $C_{21}H_{19}N_3O_3S.xCH_4O_3S$
78186-41-1 Methanesulfonamide, *N*-[4-(9-acridinylamino)phenyl]-, hydrochloride $C_{20}H_{17}N_3O_2S.xClH$
78186-42-2 Morpholinium, 4,4'-[(1,1'-biphenyl)-4,4'-diylbis(2-oxo-2,1-ethanediyl)]bis[4-ethyl-, dibromide $C_{28}H_{38}N_2O_4.2Br$
78186-43-3 Morpholine, 4-[2-[2-(2-methylnaphtho[2,3-*d*]-1,3-dioxol-2-yl)ethoxy]ethyl]-, 2-hydroxy-1,2,3-propanetricarboxylate $C_{20}H_{25}NO_4.xC_6H_8O_7$
78186-44-4 Benzenemethanol, α-[2-(diethylamino)-1-methylethyl]-3-fluoro-α-(3-fluorophenyl)-, hydrobromide $C_{20}H_{25}F_2NO.BrH$
78186-45-5 Benzenemethanol, α-[2-(diethylamino)-1-methylethyl]-4-methyl-α-(4-methylphenyl)-, hydrochloride $C_{22}H_{31}NO.ClH$
78186-46-6 Benzenemethanol, α-[2-(diethylamino)-1-methylethyl]-α-(3,4-dimethoxyphenyl)-3,4-dimethoxy- $C_{24}H_{35}NO_5$
78186-47-7 Benzenemethanol, α-[2-[[2-(dimethylamino)ethyl]methylamino]-1-methylethyl]-α-phenyl-, dihydrochloride $C_{21}H_{30}N_2O.2ClH$
78186-48-8 Benzenemethanol, α-[2-[(2-furanylmethyl)amino]-1-methylethyl]-α-phenyl- $C_{21}H_{23}NO_2$
78186-49-9 Benzenemethanol, α-[2-[(2-furanylmethyl)amino]-1-methylethyl]-α-phenyl-, (*Z*)-2-butenedioate (salt) $C_{21}H_{23}NO_2.xC_4H_4O_4$
78186-50-2 Benzenemethanol, α-[2-[(2-furanylmethylene)amino]-1-methylethyl]-α-phenyl- $C_{21}H_{21}NO_2$
78186-51-3 Benzenemethanol, α-[2-(methylamino)propyl]-α-phenyl-, hydrochloride $C_{17}H_{21}NO.ClH$
78186-52-4 Benzenemethanol, α-[1-methyl-2-[(1-methyl-4-piperidinyl)amino]ethyl]-α-phenyl-, dihydrochloride $C_{22}H_{30}N_2O.2ClH$
78186-53-5 Benzenemethanol, α-[1-methyl-2-(propylamino)ethyl]-α-phenyl-, (*Z*)-2-butenedioate (salt) $C_{19}H_{25}NO.xC_4H_4O_4$
78186-54-6 Benzeneacetic acid, α-hydroxy-α-phenyl-, 3-(dibutylamino)propyl ester $C_{25}H_{35}NO_3$
78186-55-7 1,3-Benzodioxol-5-amine, 2-methyl-2-[2-(4-morpholinyl)ethyl]-, dihydrochloride, hemihydrate $C_{14}H_{20}N_2O_3.2ClH.{}^1/_2H_2O$
78186-56-8 1,2-Ethanediamine, *N,N*-diethyl-*N'*-[1-methyl-2-(2-methyl-1,3-benzodioxol-2-yl)ethyl]- $C_{17}H_{28}N_2O_2$
78186-57-9 1,2-Ethanediamine, *N,N*-diethyl-*N'*-[1-methyl-2-(2-methyl-1,3-benzodioxol-2-yl)ethyl]-, (*Z*)-2-butenedioate (1:2) $C_{17}H_{28}N_2O_2.2C_4H_4O_4$
78186-58-0 Ethanamine, *N,N*-diethyl-2-[[2-(2-methyl-1,3-benzodioxol-2-yl)ethyl]thio]-, 2-hydroxy-1,2,3-propanetricarboxylate $C_{16}H_{25}NO_2S.xC_6H_8O_7$
78186-59-1 1-Propanamine, *N,N*-diethyl-3-[2-(2-methyl-1,3-benzodioxol-2-yl)ethoxy]-, 2-hydroxy-1,2,3-propanetricarboxylate $C_{17}H_{27}NO_3.xC_6H_8O_7$
78186-60-4 1,3-Benzodioxole-5,6-dimethanol $C_9H_{10}O_4$
78186-61-5 1,3-Benzodioxol-2-amine, *N*,2-dimethyl-, hydrochloride $C_9H_{11}NO_2.ClH$
78186-62-6 Piperazine, 1-methyl-4-[2-(2-methyl-1,3-benzodioxol-2-yl)ethyl]-, hydrochloride $C_{15}H_{22}N_2O_2.xClH$
78186-63-7 Piperidine, 1-[[2-methyl-2-[2-(1-piperidinyl)ethyl]-1,3-benzodioxol-5-yl]methyl]-, dihydrochloride, hemihydrate $C_{21}H_{32}N_2O_2.2ClH.{}^1/_2H_2O$
78186-64-8 Piperidine, 1-[3-[2-(2-methyl-1,3-benzodioxol-2-yl)ethoxy]propyl]-, hydrobromide $C_{18}H_{27}NO_3.BrH$
78186-65-9 26,12-(Epoxymethano)-12*H*-benzofuro[4',3',2':8,9,10]dibenzo[8',9':10',11'][1,6]dioxacyclododecino[3',2':3,4][2,6]benzodioxacycloundecino[11,12-*b*]quinoxaline $C_{40}H_{24}N_2O_6$
78186-66-0 Prost-13-ene-1,9-dione, 11,16-dihydroxy-1-(hydroxymethyl)-16-(1-propynyl)-, (11α,13*E*,16*R*)- $C_{24}H_{38}O_5$
78186-67-1 Prost-13-en-1-oic acid, 11-(acetyloxy)-5-bromo-6,9-epoxy-15-hydroxy-15-phenyl-, methyl ester, (6*S*,9α,11α,13*E*,15*S*)- $C_{30}H_{43}BrO_6$
78186-68-2 Prost-13-en-1-oic acid, 11-(acetyloxy)-5-bromo-6,9-epoxy-15-hydroxy-15-phenyl-, methyl ester, (6*S*,9α,11α,13*E*,15*R*)- $C_{30}H_{43}BrO_6$
78186-69-3 2*H*-Cyclopenta[*b*]furan-2-pentanoic acid, 4-formylhexahydro-*b*-iodo-, methyl ester $C_{14}H_{21}IO_4$
78186-70-6 Cyclopenta[*b*]pyran-2-butanoic acid, 5-(4-butoxy-4-methyl-3-oxo-1-pentenyl)octahydro-6-hydroxy-, methyl ester, [2*S*-[2α,4aα,5α(*E*),6β,7aα]]- $C_{23}H_{38}O_6$
78186-71-7 Prost-13-en-1-oic acid, 11-(acetyloxy)-5,9-epoxy-15-methoxy-16-methyl-, methyl ester, (5*R*,9α,11α,13*E*,15*S*,16*S*)- $C_{25}H_{42}O_6$
78186-72-8 Prost-13-en-1-oic acid, 11-(acetyloxy)-5,9-epoxy-15-methoxy-16-methyl-, methyl ester, (5*R*,9α,11α,13*E*,15*R*,16*S*)- $C_{25}H_{42}O_6$
78186-73-9 Prost-13-en-1-oic acid, 5,9-epoxy-15-ethynyl-11,15-dihydroxy-, (5*S*,9α,11α,13*E*,15*R*)- $C_{22}H_{34}O_5$
78186-74-0 Prost-13-yn-1-oic acid, 6,9-epoxy-15-methoxy-, (6*R*,9α)- $C_{21}H_{34}O_4$
78186-75-1 Prost-13-yn-1-oic acid, 6,9-epoxy-15-methoxy-, (6*S*,9α)- $C_{21}H_{34}O_4$
78186-76-2 Prost-13-yn-1-oic acid, 6,9-epoxy-15-ethoxy-11-hydroxy-16-methyl-, ethyl ester, (6*R*,9α,11α,15*S*,16*S*)- $C_{25}H_{42}O_5$
78186-77-3 Iron, hexacarbonyl[μ-[η^4:η^4-1-[3,7,8-tris(methylene)bicyclo[2.2.2]oct-5-en-2-ylidene]-2-propanone]]di-, stereoisomer $C_{20}H_{14}Fe_2O_7$
78186-78-4 2*H*-Pyrano[2'',3'':4',5']benzofuro[2',3':3,4]cyclobuta[1,2-*d*]pyrimidine-2,8,10(7b*H*,9*H*)-trione, 7a,11,11a,11b-tetrahydro-4,7a,7b-trimethyl- $C_{18}H_{16}N_2O_5$
78186-79-5 2*H*-Pyrano[2'',3'':4',5']benzofuro[3',2':3,4]cyclobuta[1,2-*d*]pyrimidine-2,9,11(7a*H*,10*H*)-trione, 7b,8,11a,11b-tetrahydro-4,7a,11a-trimethyl- $C_{18}H_{16}N_2O_5$
78186-80-8 5-Hexen-3-one, 4,4-dimethyl- $C_8H_{14}O$
78186-81-9 5-Hexen-3-one, 1-ethoxy- $C_8H_{14}O_2$
78186-82-0 Carbonotrithioic acid, 1,2-ethanediyl ester, dilithium salt $C_4H_6S_6.2Li$
78186-83-1 Carbonotrithioic acid, 2-(1,3-dithiolan-2-ylthio)ethyl methyl ester $C_7H_{12}S_6$
78186-84-2 Carbonotrithioic acid, 1,2-ethanediyl bis(phenylmethyl) ester $C_{18}H_{18}S_6$
78186-85-3 1,3-Dithiolane-2-thione, 4-ethyl- $C_5H_8S_3$
78186-86-4 Carbonotrithioic acid, butyl 2-(1,3-dithiolan-2-ylthio)ethyl ester $C_{10}H_{18}S_6$
78186-87-5 Carbonotrithioic acid, 2-(1,3-dithiolan-2-ylthio)ethyl ethyl ester $C_8H_{14}S_6$
78186-88-6 Carbonotrithioic acid, 1,2-ethanediyl dipropyl ester $C_{10}H_{18}S_6$
78186-89-7 Carbonotrithioic acid, 2-(1,3-dithiolan-2-ylthio)ethyl propyl ester $C_9H_{16}S_6$
78186-90-0 Carbonotrithioic acid, 1,2-ethanediyl dibutyl ester $C_{12}H_{22}S_6$
78186-91-1 Acetic acid, (dimethoxyphosphinyl)hydroxy-, methyl ester $C_5H_{11}O_6P$
78186-92-2 Acetic acid, (dimethoxyphosphinyl)(2-ethoxyethoxy)-, methyl ester $C_9H_{19}O_7P$
78186-93-3 Acetic acid, (dimethoxyphosphinyl)[(tetrahydro-2*H*-pyran-2-yl)oxy]-, methyl ester $C_{10}H_{19}O_7P$
78186-94-4 Acetic acid, (dimethoxyphosphinyl)(1-methoxy-1-methylethoxy)-, methyl ester $C_9H_{19}O_7P$
78186-95-5 Acetic acid, (dimethoxyphosphinyl)[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, methyl ester $C_{11}H_{25}O_6PSi$
78186-96-6 2-Pentenoic acid, 4-methyl-2-[(tetrahydro-2*H*-pyran-2-yl)oxy]-, methyl ester, (*E*)- $C_{12}H_{20}O_4$
78186-97-7 2-Pentenoic acid, 2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-methyl-, methyl ester, (*E*)- $C_{13}H_{26}O_3Si$
78186-98-8 2-Hexenoic acid, 2-(2-ethoxyethoxy)-5-methyl-, methyl ester, (*E*)- $C_{12}H_{22}O_4$
78186-99-9 2-Hexenoic acid, 2-(1-methoxy-1-methylethoxy)-5-methyl-, methyl ester, (*E*)- $C_{12}H_{22}O_4$
78187-00-5 1*H*-Pyrrole-1-carboxylic acid, 3-(2-ethoxyethoxy)-2,5-dihydro-2-oxo-5-(phenylmethyl)-, phenylmethyl ester, (±)- $C_{23}H_{25}NO_5$
78187-01-6 2-Pentenoic acid, 2-(2-ethoxyethoxy)-5-phenyl-4-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, (±)- $C_{24}H_{29}NO_6$
78187-02-7 2*H*-Pyrrol-2-one, 3-(2-ethoxyethoxy)-1,5-dihydro-5-(phenylmethyl)-, (±)- $C_{15}H_{19}NO_3$
78187-03-8 2*H*-Pyrrol-2-one, 1-acetyl-1,5-dihydro-3-hydroxy-5-(phenylmethyl)-, (±)- $C_{13}H_{13}NO_3$
78187-04-9 2-Pentenoic acid, 4-methyl-2-[(tetrahydro-2*H*-pyran-2-yl)oxy]-, methyl ester, (*Z*)- $C_{12}H_{20}O_4$
78187-05-0 2-Pentenoic acid, 2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-methyl-, methyl ester, (*Z*)- $C_{13}H_{26}O_3Si$
78187-06-1 2-Hexenoic acid, 2-(2-ethoxyethoxy)-5-methyl-, methyl ester, (*Z*)- $C_{12}H_{22}O_4$
78187-07-2 2-Hexenoic acid, 2-(1-methoxy-1-methylethoxy)-5-methyl-, methyl ester, (*Z*)- $C_{12}H_{22}O_4$
78187-08-3 Oxiranecarboximidothioic acid, 3-(2-chlorophenyl)-2-cyano-, propyl ester $C_{13}H_{13}ClN_2OS$
78187-09-4 Oxiranecarboximidic acid, 3-(2-chlorophenyl)-2-cyano-, methyl ester $C_{11}H_9ClN_2O_2$
78187-10-7 2,2-Oxiranedicarboximidic acid, 3-(2-chlorophenyl)-, dimethyl ester $C_{12}H_{13}ClN_2O_3$
78187-11-8 Oxiranecarboxamide, 3-(2-chlorophenyl)-2-cyano-, *trans*- $C_{10}H_7ClN_2O_2$
78187-12-9 Oxiranecarboxamide, 3-(2-chlorophenyl)-2-cyano-, *cis*- $C_{10}H_7ClN_2O_2$
78187-13-0 Oxiranecarboxamide, 3-(2-chlorophenyl)-2-cyano-*N*-[(2-hydroxyethoxy)methyl]-, *trans*- $C_{13}H_{13}ClN_2O_4$
78187-14-1 1,3,2-Dithiaphospholane, 2-(1,1-dimethylethyl)-, 2-oxide $C_6H_{13}OPS_2$
78187-15-2 1,3,2-Dithiaphospholane, 2-(1,1-dimethylethyl)-, 2-sulfide $C_6H_{13}PS_3$

Consult Most Recent Cumulative Registry Number Update Before Using This Handbook

78187-16-3 1,3,7,9-Tetrathia-2,8-diphosphacyclododecane, 2,8-dimethyl-, 2,8-disulfide, stereoisomer $C_8H_{18}P_2S_6$
78187-17-4 Phosphonodithious acid, (1,1-dimethylethyl)-, diethyl ester $C_8H_{19}PS_2$
78187-18-5 Benzene, 1,1'-[1,2-ethanediylbis(oxy-2,1-ethanediyloxy)]bis[4-methyl-2-nitro- $C_{20}H_{24}N_2O_8$
78187-19-6 Benzenamine, 2,2'-[1,2-ethanediylbis(oxy-2,1-ethanediyloxy)]bis[5-methyl- $C_{20}H_{28}N_2O_4$
78187-20-9 Dodecanoic acid, 5-(nitrosooxy)-, potassium salt $C_{12}H_{23}NO_4.K$
78187-21-0 Dodecanoic acid, 7-(nitrosooxy)-, potassium salt $C_{12}H_{23}NO_4.K$
78187-22-1 Dodecanoic acid, 8-(nitrosooxy)-, potassium salt $C_{12}H_{23}NO_4.K$
78187-23-2 Dodecanoic acid, 10-(nitrosooxy)-, potassium salt $C_{12}H_{23}NO_4.K$
78187-24-3 Dodecanoic acid, 12-(nitrosooxy)-, potassium salt $C_{12}H_{23}NO_4.K$
78187-25-4 Dodecanoic acid, 6-oxo-, potassium salt $C_{12}H_{22}O_3.K$
78187-26-5 Dodecanoic acid, 7-oxo-, potassium salt $C_{12}H_{22}O_3.K$
78187-27-6 Propanedioic acid, [3-acetyl-6-(1,1-dimethylethyl)-2-cyclohexen-1-yl]-, diethyl ester, *cis*- $C_{19}H_{30}O_5$
78187-28-7 Ethanone-2,2,2-*d*3, 1-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl]- $C_{12}H_{17}D_3O$
78187-29-8 Ethanone-2,2,2-*d*3, 1-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl-3-*d*]-, *trans*- $C_{12}H_{16}D_4O$
78187-30-1 Ethanone-2,2,2-*d*3, 1-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl-3,3-*d*2]- $C_{12}H_{15}D_5O$
78187-31-2 2-Cyclohexene-1-acetic acid, 3-acetyl-α-cyano-6-(1,1-dimethylethyl)-, ethyl ester $C_{17}H_{25}NO_3$
78187-32-3 Pentyl, 1-mercapto-1,3-dimethyl- $C_7H_{16}S$
78187-33-4 Sulfur, (1,1-dimethylethyl)(1,3-dimethylpentyl)hydro- $C_{11}H_{26}S$
78187-34-5 Sulfur, bis(1,1-dimethylethyl)hydrodi- $C_8H_{18}S_2$
78187-35-6 Pyrrolidine, 1,3-dimethyl-3-(1-methylethenyl)-2-(3,4,5-trimethoxyphenyl)-, *cis*- $C_{18}H_{27}NO_3$
78187-36-7 Pyrrolidine, 2-(4-chlorophenyl)-1,3-dimethyl-3-(1-methylethenyl)-, *cis*- $C_{15}H_{20}ClN$
78187-37-8 Pyrrolidine, 1,3-dimethyl-3-(1-methylethenyl)-2-(3,4,5-trimethoxyphenyl)-, hydrochloride, *cis*- $C_{18}H_{27}NO_3.ClH$
78187-38-9 Pyrrolidine, 2-(4-chlorophenyl)-1,3-dimethyl-3-(1-methylethenyl)-, hydrochloride, *cis*- $C_{15}H_{20}ClN.ClH$
78187-39-0 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-(3,4,5-trimethoxyphenyl)-, *cis*- $C_{18}H_{29}NO_3$
78187-40-3 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-(3,4,5-trimethoxyphenyl)-, hydrochloride, *cis*- $C_{18}H_{29}NO_3.ClH$
78187-41-4 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-phenyl-, *cis*- $C_{15}H_{23}N$
78187-42-5 Pyrrolidine, 1,3-dimethyl-3-(1-methylethyl)-2-phenyl-, hydrochloride, *cis*- $C_{15}H_{23}N.ClH$
78187-43-6 Piperidine, 1,3,3,4-tetramethyl-2-(3,4,5-trimethoxyphenyl)-, *cis*- $C_{18}H_{29}NO_3$
78187-44-7 Piperidine, 1,3,3,4-tetramethyl-2-(3,4,5-trimethoxyphenyl)-, hydrochloride, *cis*- $C_{18}H_{29}NO_3.ClH$
78187-45-8 Piperidine, 1,3,3,4-tetramethyl-2-phenyl-, *cis*- $C_{15}H_{23}N$
78187-46-9 Piperidine, 1,3,3,4-tetramethyl-2-phenyl-, hydrochloride, *cis*- $C_{15}H_{23}N.ClH$
78187-47-0 9-Octadecenoic acid (*Z*)-, 3-[(1-oxotetradecyl)oxy]propyl ester $C_{55}H_{68}O_4$
78187-48-1 9-Octadecenoic acid (*Z*)-, 3-[(1-oxohexadecyl)oxy]propyl ester $C_{57}H_{70}O_4$
78187-49-2 β-D-Glucopyranosiduronic acid, 1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester, 2,3,4-triacetate $C_{17}H_{20}N_2O_{10}S$
78187-50-5 β-D-Glucopyranosiduronic acid, 5-chloro-1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester, 2,3,4-triacetate $C_{17}H_{19}ClN_2O_{10}S$
78187-51-6 β-D-Glucopyranosiduronic acid, 5-bromo-1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester, 2,3,4-triacetate $C_{17}H_{19}BrN_2O_{10}S$
78187-52-7 β-D-Glucopyranosiduronic acid, 1,4-dihydro-5-iodo-4-oxo-2-pyrimidinyl 1-thio-, methyl ester, 2,3,4-triacetate $C_{17}H_{19}IN_2O_{10}S$
78187-53-8 β-D-Glucopyranosiduronic acid, 1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester $C_{11}H_{14}N_2O_7S$
78187-54-9 β-D-Glucopyranosiduronic acid, 5-chloro-1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester $C_{11}H_{13}ClN_2O_7S$
78187-55-0 β-D-Glucopyranosiduronic acid, 5-bromo-1,4-dihydro-4-oxo-2-pyrimidinyl 1-thio-, methyl ester $C_{11}H_{13}BrN_2O_7S$
78187-56-1 β-D-Glucopyranosiduronic acid, 1,4-dihydro-5-iodo-4-oxo-2-pyrimidinyl 1-thio-, methyl ester $C_{11}H_{13}IN_2O_7S$
78187-57-2 α-L-*threo*-Hex-4-enopyranosiduronic acid, 1,4-dihydro-4-oxo-2-pyrimidinyl 4-deoxy-1-thio-, methyl ester $C_{11}H_{12}N_2O_6S$
78187-58-3 α-L-*threo*-Hex-4-enopyranosiduronic acid, 5-chloro-1,4-dihydro-4-oxo-2-pyrimidinyl 4-deoxy-1-thio-, methyl ester $C_{11}H_{11}ClN_2O_6S$
78187-59-4 α-L-*threo*-Hex-4-enopyranosiduronic acid, 5-bromo-1,4-dihydro-4-oxo-2-pyrimidinyl 4-deoxy-1-thio-, methyl ester $C_{11}H_{11}BrN_2O_6S$

95: 41674c **Mass-spectroscopic study of optical whiteners. V. Mass spectra of derivatives of benzo- and naphthotriazoles.** Shibryaeva, L. S.; Ushakova, R. L.; Mikaya, A. I.; Zaikin, V. G. (Nauchno-Issled. Inst. Poluprod. Krasitelei, Moscow, USSR). *Zh. Obshch. Khim.* 1981, 51(2), 447-51 (Russ). The mass



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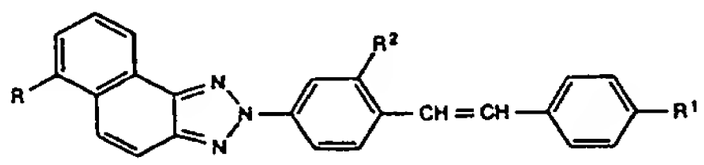
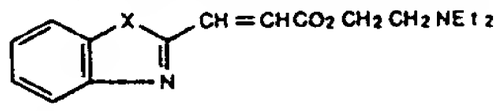


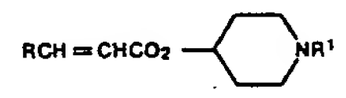
II

spectra of **I** and **II** [R = H, SO_2OPh; R^1 = H, Cl; R^2 = CN, SO_2OPh, $SO_2NH(CH_2)_3NMe_2$] indicated that the main fragmentation involved loss of N_2H. For compds. contg. the SO_2OPh group, intense peaks corresponding to loss or fragmentation of this group were obsd.

95: 41675d **Proton magnetic resonance of some acrylic esters.** Ibrahim, E. H. M.; Abdel Rahman, M. O.; Abdellah, I. M. (Fac. Sci., Al-Azhar Univ., Cairo, Egypt). *Egypt. J. Chem.* 1979 (Pub. 1980). 22(4), 265-71 (Eng). The ^1H NMR of **I** (X



I

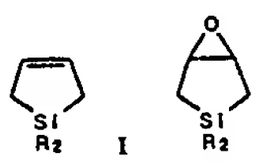


II

= O, S) and **II** (R = 2-furyl, R^1 = Me; R = 2-benzothiazolyl, R^1 = Et) were obsd. in CCl_4.

95: 41676e **GC/MS analysis of some long chain esters, ketones and propanediol diesters.** Vajdi, M.; Nawar, W. W.; Merritt, C., Jr. (Dep. Food Sci. Nutr., Univ. Massachusetts, Amherst, MA 01003 USA). *J. Am. Oil Chem. Soc.* 1981, 58(2), 106-10 (Eng). In the title study, double hydrogen rearrangement led to the predominant ion in the spectrum of long-chain satd. esters: in the unsatd. esters, a peak corresponding to the loss of alc. from the mol. ion was more pronounced. In contrast to short-chain ketones, McLafferty rearrangement was not the major fragmentation in the spectrum of satd. and unsatd. long-chain ketones. α-Cleavage was the predominant fragmentation in the spectrum of these ketones. The McLafferty + 1 rearrangement peak was more pronounced for the long-chain ketones than for smaller ketones. Fragmentation patterns of propanediol diesters were similar to those in triglycerides, giving rise to predominant peaks corresponding to acylium ion $[RCO]^+$ and parent minus acyloxy ion $[RCOO]^+$.

95: 41677f **Carbon-13 NMR spectra of 1,1-disubstituted 1-sila-3-cyclopentenes and their 3,4-epoxy derivatives.** Panasenko, A. A.; Khalilov, L. M.; Tsyrlina, E. M.; Yur'ev, V. P. (Inst. Khim., Ufa, USSR). *Izv. Akad. Nauk SSSR, Ser. Khim.* 1981, (2), 424-7 (Russ). ^{13}C NMR data were obtained



I

II

for **I** (R = Me, Ph, $OSiMe_3$, $OCHMe_2$, OMe, OEt, Cl) and **II** (R = Me, Ph, $OSiMe_3$, $OCHMe_2$, $OCMe_3$). The shielding effect of the epoxy ring was manifested in the magnetic nonequivalence of the Me carbons of the $CHMe_2$ and CMe_3 groups.

95: 41678g **Electron impact fragmentation of alkoxymethylsilylamines.** Pikies, J.; Wojnowski, W.; Meller, A. (Inst. Inorg. Chem. Technol., Tech. Univ., Gdansk, Pol.). *Z. Anorg. Allg. Chem.* 1981, 473, 215-23 (Ger). The mass spectra of the following compds. were recorded (R = Bu, Ph): $(Me_3CO)_3SiNHR$, $(Me_2CHO)_3SiNHR$, $(Me_2CHO)_2SiMeNHR$, $Me_2CHOSiMe_2NHR$, Me_3SiNHR. The *N*-Bu compds. underwent a rearrangement in which H migrated to the siliconium center. With the *N*-Ph compds. the mol. ion and other radical ions exhibited remarkably high stability. A new rearrangement of the NHPh group was obsd.

95: 41679h **NMR spectroscopic studies of boron compounds. XIX. Carbon-13 NMR studies on monoaminoboranes and borazines.** Noeth, Heinrich; Wrackmeyer, Bernd (Inst. Anorg. Chem., Univ Muenchen, D-8000 Munich, 2 Fed. Rep. Ger.). *Chem. Ber.* 1981, 114(3), 1150-6 (Ger). Chem. shifts $\delta(^{13}C)$ of $R_2BNR^1_2$ and $X_2BNR^1_2$ and of borazines $(RBNR^1)_3$ and $(XBNR^1)_3$ (X = halo, OR, SR, NR_2) are related to a γ-effect exerted by R and X on the shielding of ^{13}C(BC) and ^{13}C(NC). Analogies exist with similar effects in alkenes, immonium salts, and C_6H_6 derivs. Heteronuclear ^{13}C $\{^1H,^{11}B\}$ triple-resonance expts. permit the observation of sharp ^{13}C(BC) resonance signals.

95: 41680b **Reaction of cyclohexanone with ammonium ion under chemical ionization conditions. 1. Formation of protonated unsubstituted imines.** Tabet, J. C.; Fraisse, D. (Lab. Synth. Org., Ec. Polytech., 91128 Palaiseau, Fr.). *Org. Mass Spectrom.* 1981, 16(1), 45-7 (Eng). High resoln. and metastable decompn. spectra were recorded of the ions $[M + NH_4]^+$ formed by reaction of NH_4^+ with cyclohexanone. The *m/z* 98 ion, abundant in the NH_3 chem. ionization spectrum of cyclohexanone, is composed of 2 isobaric ions: a protonated imine ion and the mol. ion of cyclohexanone. The former is formed by a process analogous to that which occurs in soln.

95: 41681c **The mass spectra of some substituted methyl cinnamates.** Zalewski, Romuald I. (Dep. Chem., Univ. Sulaimanyiah, Sulaimanyiah, Iraq). *Org. Mass Spectrom.* 1981, 16(1), 52 (Eng). The mass spectra were recorded of $RC_6H_4CH{:=}CHCO_2Me$ (R = H, 4-OH, 3-OH, 4-Me, 3-Cl, 4-Cl, 3-Br, 3-NO_2, 4-NO_2). A parent ion of high intensity (40-80%) was present in all spectra and was accompanied by $[M+1]^{\bullet+}$ and $[M-1]^{\bullet+}$ peaks. The base peak was in all cases $[M-31]^{\bullet+}$ (**I**), formed by loss of OMe•. **I** loses CO to give the ion $[M-59]^{\bullet+}$ which decomps. in a typical way for an arom. moiety to give a variety of peaks below *m/z* 93.

95: 41682d **Microwave spectra of dimethyl sulfide-d_6, $(CD_3)_2S$, ground and excited torsional states.** Demaison, Jean; Tan, B. T.; Typke, V.; Rudolph, H. D. (Dep. Phys., Univ. Lille I, F-59655 Villeneuve d'Ascq, Fr.). *J. Mol. Spectrosc.* 1981, 86(2), 406-19 (Eng). The microwave spectra of $(CD_3)_2S$ in the ground state and 1st and 2nd excited states of Me-top torsion (internal rotation) and of CSC deformation as well as the ground-state spectra of the ^{13}C- and ^{34}S-substituted forms were measured. The rotational consts. and centrifugal-distortion and rotation-vibration interaction consts. were detd. The rotational lines in the excited torsional states (1_1, 1_2, 2_1, 2_2, 2_3) were split into quartets, owing to the interaction between mol. rotation and Me-top internal rotation. The exptl. multiplet splittings were fitted to those calcd. from a rotation-internal rotation Hamiltonian in order to obtain values for the internal-rotation barrier V_3 and the top-top interaction potential coeffs. V_{12} and V'_{12}; V_{12} was too highly correlated with V_3 for a sep. detn. The values following from the least-squares adjustment are discussed.

95: 41683e **Acetic acid: microwave spectra, internal rotation and substitution structure.** Van Eijck, B. P.; Van Opheusden, J.; Van Schaik, M. M. M.; Van Zoeren, E. (Dep. Struct. Chem., Univ. Utrecht, 3584 CH Utrecht, Neth.). *J. Mol. Spectrosc.* 1981, 86(2), 465-79 (Eng). The internal-rotation splittings in the microwave spectrum of AcOH were reexamd., using both principal-axis method (PAM) and internal-axis method (IAM) treatments. Individual terms in the PAM equation correlated with the 1st terms in an expansion of the corresponding IAM formula. When centrifugal distortion was allowed for, both methods reproduced the *A*-type frequencies within exptl. error. To derive the substitution structure, 8 isotopic species were studied. The inertial moments of the mols. with various degrees of Me-group deuteration are not consistent with each other, so these data could not be fully used. Therefore, the structure was derived with the assumption of a cylindrically sym. Me group, although there is some evidence that the HCH angles differ by a few degrees. The geometry, which agrees with earlier electron-diffraction results, is compared with the substitution structures of other carboxylic acids.

95: 41684f **Refinements of mass spectrometry/mass spectrometry and applications to organic analysis.** Sigsby, Mary Lou (Purdue Univ., West Lafayette, IN USA). 1980. 226 pp. (Eng). Avail. Univ. Microfilms Int., Order No. 8102708. From *Diss. Abstr. Int. B* 1981, 41(8), 3022.

95: 41685g **Spectral characteristics of drugs with an oxygen heteroatom.** Buryak, V. P. (Med. Inst., Zaporozhe, USSR). *Farm. Zh. (Kiev)* 1981, (1), 68-9 (Ukrain). The UV spectrum of khellin has absorption max. at 242-51, 280-4 and 320-37 nm, the last one being the most characteristic of furochromone systems and corresponding to a $\pi-\pi^*$ transition.

95: 41686h **$C_3H_3^+$ in flames and the proton affinity of cyclopropenylidene or propadienylidene (C_3H_2).** McAllister, Trevor; Nicholson, Anthony J. C. (Div. Chem. Phys., CSIRO, Clayton, 3168 Australia). *J. Chem. Soc., Faraday Trans. 1* 1981, 77(4), 821-5 (Eng). $C_3H_3^+$ was prominent in the reaction zone of a CH_4 + Ar flame, but was displaced by NH_4^+ when NH_3 was added. These observations were explained in terms of the equil. in the proton-transfer reactions $H_3O^+ + C_3H_2 \leftrightarrow C_3H_3^+ + H_2O$ (*A*) and $NH_4^+ + C_3H_2 \leftrightarrow C_3H_3^+ + NH_3$ (*B*). In reaction *A*, the proton affinity of C_3H_2 is much greater than that of H_2O, leading to H_3O^+ formation in substantial amts. only when the H_2O concn. is several orders of magnitude larger than that of C_3H_2. In reaction *B*, the higher proton affinity of NH_3 ensures that NH_4^+ dominates the reaction zone. Ion-cyclotron-resonance expts. showed that the proton affinity of C_3H_2 is >65 kJ/mol greater than that of NH_3. The concn. of C_3H_2 in the reaction zone was estd. as 7×10^{12} cm^{-3} lower than the detection limit of mass spectrometry.

95: 41687j **Fast searching for identical carbon-13 NMR spectra via inverted files.** Bremser, W.; Wagner, H.; Franke, B. (Cent. Res., BASF A.-G., D-6700 Ludwigshafen, Fed. Rep. Ger.). *Org. Magn. Reson.* 1981, 15(2), 178-87 (Eng). For large mols. and incomplete spectra, computer matching of